Shantenu Jha

List of Publications by Year in descending order

91 papers	1,687 citations	393982 19 h-index	414034 32 g-index
97 all docs	97 docs citations	97 times ranked	1921 citing authors

#	Article	IF	Citations
1	Design and Performance Characterization of RADICAL-Pilot on Leadership-Class Platforms. IEEE Transactions on Parallel and Distributed Systems, 2022, 33, 818-829.	4.0	18
2	High-Throughput Virtual Screening and Validation of a SARS-CoV-2 Main Protease Noncovalent Inhibitor. Journal of Chemical Information and Modeling, 2022, 62, 116-128.	2.5	54
3	A new hourly dataset for photovoltaic energy production for the continental USA. Data in Brief, 2022, 40, 107824.	0.5	3
4	Coupling streaming AI and HPC ensembles to achieve 100â€“1000Ã— faster biomolecular simulations. , 2022, , .		4
5	AI-driven multiscale simulations illuminate mechanisms of SARS-CoV-2 spike dynamics. International Journal of High Performance Computing Applications, 2021, 35, 432-451.	2.4	91
6	Pilot-Edge: Distributed Resource Management Along the Edge-to-Cloud Continuum. , 2021, , .		11
7	Scalable HPC & AI infrastructure for COVID-19 therapeutics. , 2021, , .		12
8	Comparing workflow application designs for high resolution satellite image analysis. Future Generation Computer Systems, 2021, 124, 315-329.	4.9	1
9	Dynamic and Adaptive Monitoring and Analysis for Many-task Ensemble Computing. , 2021, , .		0
10	Pandemic drugs at pandemic speed: infrastructure for accelerating COVID-19 drug discovery with hybrid machine learning- and physics-based simulations on high-performance computers. Interface Focus, 2021, 11, 20210018.	1.5	23
11	A Community Roadmap for Scientific Workflows Research and Development. , 2021, , .		14
12	Extensible and Scalable Adaptive Sampling on Supercomputers. Journal of Chemical Theory and Computation, 2020, 16, 7915-7925.	2.3	14
13	Methods and Experiences for Developing Abstractions for Data-intensive, Scientific Applications. , 2020, , .		0
14	Parallel performance of molecular dynamics trajectory analysis. Concurrency Computation Practice and Experience, 2020, 32, e5789.	1.4	1
15	Adaptive Ensemble Biomolecular Applications at Scale. SN Computer Science, 2020, 1, 1.	2.3	14
16	ICEBERG: Imagery Cyber-infrastructure and Extensible Building blocks to Enhance Research in the Geosciences. (A Research Programmerâ€™s Perspective). , 2020, , .		0
17	A Comprehensive Perspective on Pilot-Job Systems. ACM Computing Surveys, 2019, 51, 1-32.	16.1	36
18	Middleware Building Blocks for Workflow Systems. Computing in Science and Engineering, 2019, 21, 62-75.	1.2	19

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19	Supporting High-Performance and High-Throughput Computing for Experimental Science. Computing and Software for Big Science, 2019, 3, 1.	1.3	9
20	Understanding ML Driven HPC: Applications and Infrastructure. , 2019, , .		2
21	Characterizing the Performance of Executing Many-tasks on Summit. , 2019, , .		8
22	Learning Everywhere: A Taxonomy for the Integration of Machine Learning and Simulations. , 2019, , .		5
23	Workflow Design Analysis for High Resolution Satellite Image Analysis. , 2019, , .		4
24	DeepDriveMD: Deep-Learning Driven Adaptive Molecular Simulations for Protein Folding. , 2019, , .		42
25	CoCo-MD: A Simple and Effective Method for the Enhanced Sampling of Conformational Space. Journal of Chemical Theory and Computation, 2019, 15, 2587-2596.	2.3	20
26	Using Pilot Systems to Execute Many Task Workloads on Supercomputers. Lecture Notes in Computer Science, 2019, , 61-82.	1.0	13
27	HPC enabled parallel, multi-scale & mechanistic model for high shear granulation using a coupled DEM-PBM framework. Computer Aided Chemical Engineering, 2018, 44, 1459-1464.	0.3	1
28	Concurrent and Adaptive Extreme Scale Binding Free Energy Calculations. , 2018, , .		7
29	High-throughput binding affinity calculations at extreme scales. BMC Bioinformatics, 2018, 19, 482.	1.2	14
30	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	1.2	72
31	Pilot-Streaming: A Stream Processing Framework for High-Performance Computing. , 2018, , .		7
32	Adaptive ensemble simulations of biomolecules. Current Opinion in Structural Biology, 2018, 52, 87-94.	2.6	24
33	A parallel unidirectional coupled DEM-PBM model for the efficient simulation of computationally intensive particulate process systems. Computers and Chemical Engineering, 2018, 119, 128-142.	2.0	9
34	Harnessing the Power of Many: Extensible Toolkit for Scalable Ensemble Applications. , 2018, , .		26
35	Synapse: Synthetic application profiler and emulator. Journal of Computational Science, 2018, 27, 329-344.	1.5	5
36	A Systematic Framework for Data Management and Integration in a Continuous Pharmaceutical Manufacturing Processing Line. Processes, 2018, 6, 53.	1.3	19

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37	Task-parallel Analysis of Molecular Dynamics Trajectories. , 2018, , .		8
38	On the complexities of utilizing largeâ€scale lightpathâ€connected distributed cyberinfrastructure. Concurrency Computation Practice and Experience, 2017, 29, e3853.	1.4	2
39	Introducing distributed dynamic dataâ€intensive (D3) science: Understanding applications and infrastructure. Concurrency Computation Practice and Experience, 2017, 29, e4032.	1.4	4
40	Conceptualizing a Computing Platform for Science Beyond 2020: To Cloudify HPC, or HPCify Clouds?. , 2017, , .		4
41	Hacking at the Divide Between Polar Science and HPC: Using Hackathons as Training Tools. , 2017, , .		5
42	High-Throughput Computing on High-Performance Platforms: A Case Study. , 2017, , .		11
43	Evaluating Distributed Execution of Workloads. , 2017, , .		6
44	ExTASY: Scalable and flexible coupling of MD simulations and advanced sampling techniques. , 2016, , .		15
45	A Scalable Pipeline for Transcriptome Profiling Tasks with On-Demand Computing Clouds. , 2016, , .		0
46	Integrating Abstractions to Enhance the Execution of Distributed Applications. , 2016, , .		6
47	RepEx: A Flexible Framework for Scalable Replica Exchange Molecular Dynamics Simulations. , 2016, , .		6
48	Synapse: Synthetic Application Profiler and Emulator. , 2016, , .		2
49	Ensemble Toolkit: Scalable and Flexible Execution of Ensembles of Tasks. , 2016, , .		20
50	Application skeletons: Construction and use in eScience. Future Generation Computer Systems, 2016, 59, 114-124.	4.9	8
51	Application Skeleton: Generating Synthetic Applications for Infrastructure Research. Journal of Open Source Software, 2016, 1, 17.	2.0	1
52	Characterization of the Three-Dimensional Free Energy Manifold for the Uracil Ribonucleoside from Asynchronous Replica Exchange Simulations. Journal of Chemical Theory and Computation, 2015, 11, 373-377.	2.3	10
53	SAGA: A standardized access layer to heterogeneous Distributed Computing Infrastructure. SoftwareX, 2015, 1-2, 3-8.	1.2	27
54	Pilot-Data: An abstraction for distributed data. Journal of Parallel and Distributed Computing, 2015, 79-80, 16-30.	2.7	7

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55	Developing eThread Pipeline Using SAGA-Pilot Abstraction for Large-Scale Structural Bioinformatics. BioMed Research International, 2014, 2014, 1-12.	0.9	5
56	Comparative analysis of nucleotide translocation through protein nanopores using steered molecular dynamics and an adaptive biasing force. Journal of Computational Chemistry, 2014, 35, 692-702.	1.5	23
57	Advancing nextâ€generation sequencing data analytics with scalable distributed infrastructure. Concurrency Computation Practice and Experience, 2014, 26, 894-906.	1.4	4
58	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	2.3	123
59	Numerical methodologies for investigation of moderate-velocity flow using a hybrid computational fluid dynamics â€" molecular dynamics simulation approach. Journal of Mechanical Science and Technology, 2014, 28, 245-253.	0.7	3
60	A Tale of Two Data-Intensive Paradigms: Applications, Abstractions, and Architectures. , 2014, , .		54
61	Towards an Understanding of Facets and Exemplars of Big Data Applications. , 2014, , .		14
62	Distributed computing practice for largeâ€scale science and engineering applications. Concurrency Computation Practice and Experience, 2013, 25, 1559-1585.	1.4	15
63	The Impact of a Ligand Binding on Strand Migration in the SAM-I Riboswitch. PLoS Computational Biology, 2013, 9, e1003069.	1.5	25
64	Exploring Dynamic Enactment of Scientific Workflows Using Pilot-Abstractions. , 2013, , .		1
65	Running many molecular dynamics simulations on many supercomputers. , 2012, , .		7
66	Distributed Application Runtime Environment (DARE): A Standards-based Middleware Framework for Science-Gateways. Journal of Grid Computing, 2012, 10, 647-664.	2.5	25
67	P∗: A model of pilot-abstractions. , 2012, , .		22
68	Conformational Heterogeneity of the SAM-I Riboswitch Transcriptional ON State: A Chaperone-Like Role for S-Adenosyl Methionine. Journal of Molecular Biology, 2012, 418, 331-349.	2.0	18
69	Characterizing deep sequencing analytics using BFAST. , 2011, , .		7
70	Autonomic Management of Application Workflows on Hybrid Computing Infrastructure. Scientific Programming, 2011, 19, 75-89.	0.5	41
71	Energy landscape analysis for regulatory RNA finding using scalable distributed cyberinfrastructure. Concurrency Computation Practice and Experience, 2011, 23, 2292-2304.	1.4	8
72	Understanding application-level interoperability: Scaling-out MapReduce over high-performance grids and clouds. Future Generation Computer Systems, 2011, 27, 590-599.	4.9	20

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73	A practical and comprehensive graduate course preparing students for research involving scientific computing. Procedia Computer Science, 2011, 4, 1927-1936.	1.2	4
74	Understanding performance of distributed data-intensive applications. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2010, 368, 4089-4102.	1.6	4
75	Exploring the RNA folding energy landscape using scalable distributed cyberinfrastructure. , 2010, , .		8
76	Exploring the Performance Fluctuations of HPC Workloads on Clouds. , 2010, , .		39
77	Efficient Runtime Environment for Coupled Multi-physics Simulations: Dynamic Resource Allocation and Load-Balancing. , 2010, , .		21
78	Abstractions for Loosely-Coupled and Ensemble-Based Simulations on Azure. , 2010, , .		12
79	SAGA BigJob: An Extensible and Interoperable Pilot-Job Abstraction for Distributed Applications and Systems. , 2010, , .		46
80	A mechanism for S-adenosyl methionine assisted formation of a riboswitch conformation: a small molecule with a strong arm. Nucleic Acids Research, 2009, 37, 6528-6539.	6.5	44
81	Using clouds to provide grids with higher levels of abstraction and explicit support for usage modes. Concurrency Computation Practice and Experience, 2009, 21, 1087-1108.	1.4	55
82	Determination of Free Energy Profiles for the Translocation of Polynucleotides through Î±-Hemolysin Nanopores using Non-Equilibrium Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 2135-2148.	2.3	33
83	An Autonomic Approach to Integrated HPC Grid and Cloud Usage. , 2009, , .		36
84	A Fresh Perspective on Developing and Executing DAG-Based Distributed Applications: A Case-Study of SAGA-Based Montage. , 2009, , .		7
85	An innovative application execution toolkit for multicluster grids. , 2009, , .		2
86	Adaptive distributed replicaâ€“exchange simulations. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2009, 367, 2595-2606.	1.6	15
87	Distributed Replica-Exchange Simulations on Production Environments Using SAGA and Migol. , 2008, , .		5
88	Rapid, Accurate, and Precise Calculation of Relative Binding Affinities for the SH2 Domain Using a Computational Grid. Journal of Chemical Theory and Computation, 2007, 3, 1193-1202.	2.3	16
89	NEKTAR, SPICE and Vortonics: using federated grids for large scale scientific applications. Cluster Computing, 2007, 10, 351-364.	3.5	22
90	SAGA: A Simple API for Grid Applications. High-level application programming on the Grid. Computational Methods in Science and Technology, 2006, 12, 7-20.	0.3	77

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91	Force field validation for nucleic acid simulations: Comparing energies and dynamics of a DNA dodecamer. Journal of Computational Chemistry, 2005, 26, 1617-1627.	1.5	17